REMARKS

The Office Action states that the Appendix is objected to. The applicant has attached papers evidencing that the Appendix has already been submitted on microfiche.

In one aspect of the invention, a method for use in deriving a chemical structure diagram includes identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure. The method further includes representing the instance of symmetry as a list of groups of equivalent atoms and bonds, and expressing the instance of chemical structural symmetry in the chemical structure diagram.

New dependent claims 13-27 have been added. Support may be found in the specification at least at pages 7-9.

All of the independent claims (1-12) have been amended. Independent claims 1, 5, 9 have been amended to recite representing the instance of symmetry as a list of groups of equivalent atoms and bonds. Support may be found in the specification at least at page 7, lines16-18.

Independent claims 2, 6, 10 have been amended to recite that the force term is based on the difference between an optimal angle and a current angle. Support may be found in the specification at least at page 12, line 9.

Independent claims 3, 7, 11 have been amended to recite that the addition includes a bridge addition to the first chemical structure diagram. Support may be found in the specification at least at page 14, lines 17-19.

Independent claims 4, 8, 12 have been amended to recite keeping track of unused display area, within which the first portion of the available layout area is defined. Support may be found in the specification at least at page 17, lines 6-7.

Claims 1-12 have been rejected over U.S. Patent No. 5,434,796 to Weininger ("Weininger"). However, it is respectfully submitted that this rejection should be withdrawn.

Weininger describes a method of and apparatus for evolving successive populations of molecular structures and evaluating each evolved structure of each population with desired physical and/or theoretical properties. An initial population of molecules is provided in terms of representations of a number of member molecules. Evaluation is performed by a fitness function, which compares the initial population and evolved generations of member representations with the set of desired properties to provide a numerical measure or value of fitness for each structure. That numerical value indicates how closely the compared member representation corresponds with the set of desired properties. The next population is generated by changing the structure of selected molecules of a population dependent upon the numerical measure of fitness, and the process repeats. Subsequent populations evolve towards ever-better fitness. The process is terminated when an acceptable molecule evolves.

Independent claims 1, 5, 9 have been rejected over Weininger. However, Weininger neither discloses nor suggests identifying an instance of symmetry and representing the instance of symmetry as a list of groups of equivalent atoms and bonds as required by amended claims 1, 5, 9.

Independent claims 2, 6, 10 have been rejected over Weininger. However, Weininger neither discloses nor suggests that a force term be based on the difference between an optimal angle and a current angle as required by amended claims 2, 6, 10.

Independent claims 3, 7, 11 have been rejected over Weininger. However, Weininger neither discloses nor suggests that an addition includes a bridge addition to a first chemical structure diagram as required by amended claims 3, 7, 11.

Independent claims 4, 8, 12 have been rejected over Weininger. However, Weininger neither discloses nor suggests keeping track of unused display area, within which the first portion of the available layout area is defined as required by amended claims 4, 8, 12.

Claims 1-12 have also been rejected as being anticipated by Applicant's Own Admission, and states "See specification Page 4, lines 1-7". However, the Office Action does not explain how the cited passage would anticipate any of the pending claims, and it is respectfully

submitted that any related rejection should be withdrawn. The applicant submits herewith a copy of the pages 313-398 cited at specification page 4, lines 1-7, and a Wiley-VCH listing evidencing that these pages were published June 1999, which is after the February 11, 1999 application date of U.S. Provisional Application Serial No. 60/119,654 ("provisional application"), the benefit of which is claimed on page 1 of the specification. It is plain from the provisional application and pages 313-398 that anything in pages 313-398 that bears on the patentability of the pending claims is predated by the provisional application.

The Office Action states "Also see Appendix Page 1, for" multiple identified pieces of software material dated 7/19/96. However, the Office Action does not explain how the material dated 7/19/96 would anticipate any of the pending claims, and it is respectfully submitted that any related rejection should be withdrawn. The applicant, who obtained his Ph.D. from Purdue University and has authored or co-authored articles on the subject of chemical structure diagram generation, is currently a developer with CambridgeSoft Corporation of Cambridge, Massachusetts, where he has worked since 1994. He is familiar with CambridgeSoft products from 1996 to the current time, including any such products that have included chemical structure diagram generation capabilities, and he is familiar with the inner workings of such capabilities. He is familiar with the Office Action dated Jan. 15, 2003, which cites the material dated 7/19/96, and confirms that the methods, systems, and software of the pending claims are not described by any of the cited 7/19/96 material.

The dependent claims are patentable for at least the same reasons stated above.

The applicant submits that the application is in condition for allowance, which action is requested. In the interest of expediting prosecution, in the event there are questions concerning the specification or claims, or concerning any of the explanations stated above, the applicant encourages the examiner to contact the undersigned directly at the telephone number given below.

The Commissioner is hereby authorized to charge any fee deficiency, or credit any overpayment to our Deposit Account No. 08-0219.

Respectfully submitted,

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Replacement Pages for Claims 1-27

(MARKED TO SHOW CHANGES)

1. A method for use in deriving a chemical structure diagram, comprising:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

representing the instance of symmetry as a list of groups of equivalent atoms and bonds; and

expressing the instance of chemical structural symmetry in the chemical structure diagram.

2. A method for use in deriving a chemical structure diagram, comprising:

determining, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

applying the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

3. A method for use in deriving a chemical structure diagram, comprising:

determining, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram;

producing the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram; and

producing a second chemical structure diagram by adding the addition to the first chemical structure diagram.

4. A method for use in deriving a chemical structure diagram, comprising:

keeping track of unused display area;

determining a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram;

determining a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

positioning the first and second chemical structure diagrams within the first and second portions, respectively.

5. A system for use in deriving a chemical structure diagram, comprising:

an identifier identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

a representor representing the instance of symmetry as a list of groups of equivalent atoms and bonds; and

an expressor expressing the instance of chemical structural symmetry in the chemical structure diagram.

6. A system for use in deriving a chemical structure diagram, comprising:

a determiner determining, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

an applicator applying the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

7. A system for use in deriving a chemical structure diagram, comprising:

a determiner determining, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram; and

a producer producing the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram, and producing a second chemical structure diagram by adding the addition to the first chemical structure diagram.

8. A system for use in deriving a chemical structure diagram, comprising:

a tracker keeping track of available display area;

a determiner determining a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram, the determiner determining a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

a positioner positioning the first and second chemical structure diagrams within the first and second portions, respectively.

9. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

identify, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

represent the instance of symmetry as a list of groups of equivalent atoms and bonds; and

express the instance of chemical structural symmetry in the chemical structure diagram.

10. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

determine, from a first chemical structure diagram, a force term for increasing diagrammatic symmetry within the first chemical structure diagram, the force term being based on the difference between an optimal angle and a current angle; and

apply the force term in a derivation of a second chemical structure diagram from the first chemical structure diagram, the second chemical structure diagram having more diagrammatic symmetry than the first chemical structure diagram.

11. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

determine, from a first chemical structure diagram, a parameter for use in producing the shape of an addition to the first chemical structure diagram;

produce the shape of the addition based on the parameter, the addition including a bridge addition to the first chemical structure diagram; and

produce a second chemical structure diagram by adding the addition to the first chemical structure diagram.

12. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

keep track of unused display area;

determine a first rectangle that defines a first portion of an available layout area within the unused display area, the first rectangle being of a sufficient size to enclose a first chemical structure diagram;

determine a second rectangle that defines a second portion of an available layout area, the second portion being non-overlapping with the first portion, the second rectangle being of a sufficient size to enclose a second chemical structure diagram; and

position the first and second chemical structure diagrams within the first and second portions, respectively.

13. The method of claim 1, wherein the instance of chemical structural symmetry is based on rotational symmetry.

14. The method of claim 1, wherein the instance of chemical structural symmetry is based on reflective symmetry.

15. The method of claim 1, wherein the instance of chemical structural symmetry is based on inversive symmetry.

16. The method of claim 1, further comprising:

basing the identification on stereochemistry.

17. The method of claim 1, further comprising:

basing the identification on rotational symmetry, reflective symmetry, and stereochemistry.

18. The method of claim 1, further comprising:

basing the identification on double bond stereochemistry.

19. The method of claim 1, further comprising:

determining a pivot point for the list.

20. The method of claim 1, further comprising:

determining a graph-theoretic center for the list.

21. The method of claim 1, further comprising:

determining a symmetric order for the instance of chemical structural symmetry.

22. The method of claim 1, further comprising:

determining whether an atom belongs to the determined instance of chemical structural symmetry.

23. The method of claim 1, further comprising:

determining whether a bond belongs to the determined instance of chemical structural symmetry.

24. The method of claim 1, further comprising:

in the event the determined instance of chemical structural symmetry is reflective, selecting a position on an opposite side of a mirror line.

25. The method of claim 1, further comprising:

in the event the determined instance of chemical structural symmetry is rotative, selecting a position based on a pivot point.

26. The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is horizontal.

27. The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is vertical.